Supporting Information

for

Oxygen-Incorporated 3D flower-like MoS_2 microsphere as a bifunctional catalyst for effectively synthesis of 2,5-diformyfuran from fructose

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Contents:

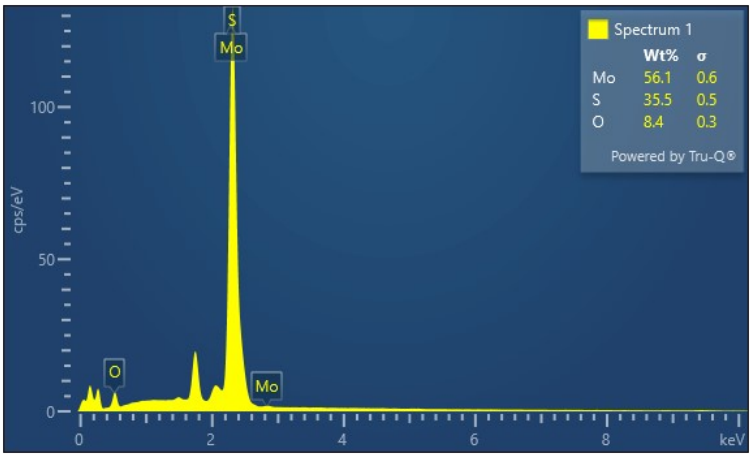

Figure S1. The EDS quantitative analysis result of the as-prepared oxygen-incorporated 3D flower-like MoS_2 microspheres.

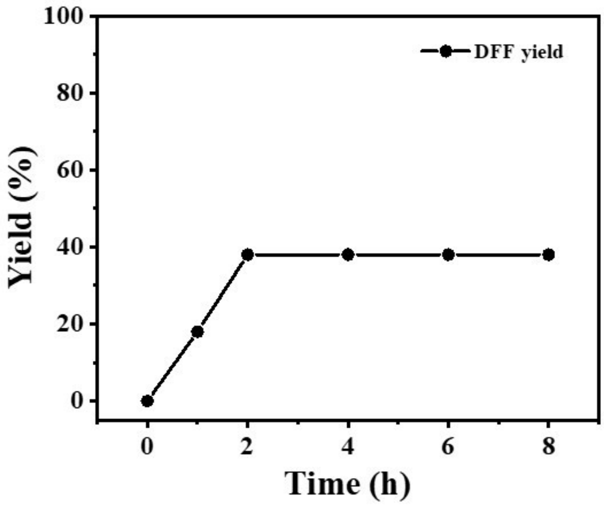

Figure S2. Leaching experiments at the optimum conditions for the oxidation of HMF to DFF catalyzed by MoS_2. Reaction conditions: HMF 0.126 g (1 mmol), MoS_2 50 mg, DMSO 4 mL, 120 °C.

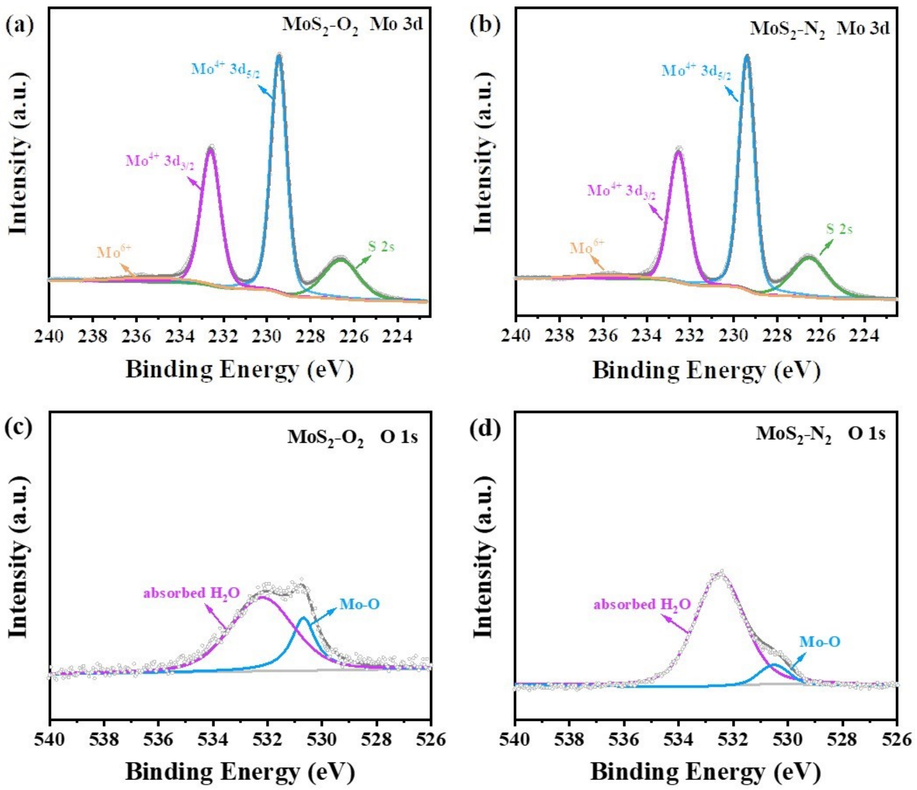

Figure S3. The high-resolution Mo 3d spectra of (a) MoS_2-O_2 and (b) MoS_2-N_2, and the high-resolution O 1s spectra of (c) MoS_2-O_2 and (d) MoS_2-N_2.

Table S1. The contents of Mo^{4+} and Mo^{6+} species, and O_α and O_β species on the surface of fresh MoS_2, MoS_2-O_2 and MoS_2-N_2.

Entry	Catalyst	Mo^{4+} (%)	Mo^{6+} (%)	O_α	O_β
1	fresh MoS_2	95.68	4.32	0.74	0.26
2	MoS_2-O_2	95.79	4.21	0.24	0.76
3	MoS_2-N_2	96.64	3.36	0.09	0.91

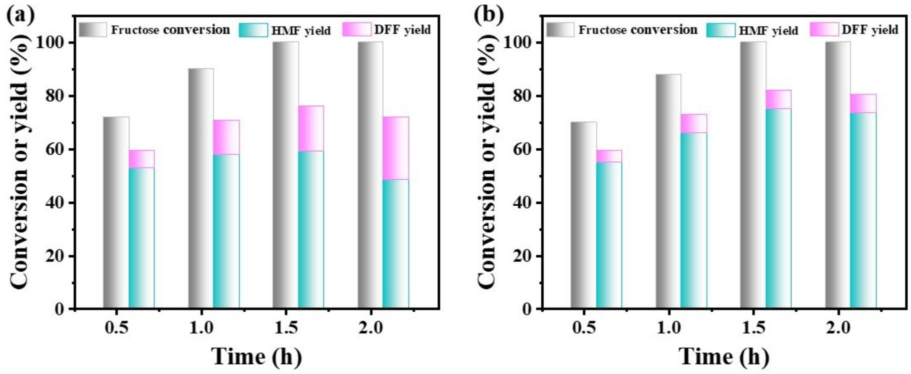

Figure S4. The results of MoS_2-catalyzed dehydration of fructose to HMF under (a) O_2 and (a) N_2 atmosphere. Reaction conditions: fructose 0.180 g (1 mmol), MoS_2 50 mg, DMSO 4 mL, 120 °C.

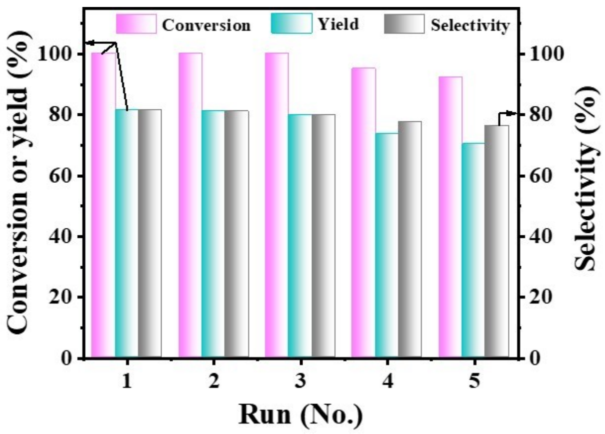

Figure S5. Recycled experiments under the optimal conditions for one-pot conversion of fructose to DFF catalyzed by MoS_2. Reaction conditions: fructose (1 mmol), MoS_2 (50 mg), DMSO (4 mL), N_2 flow rate (20 mL min^{-1}), O_2 flow rate (20 mL min^{-1}), temperature/time: 120 °C/6h.

Table S5. Comparison of the as-prepared MoS_2 catalyst with literature reported bifunctional catalysts for "one-pot" synthesis of DFF from fructose.

Entry	Catalyst	Oxidant	Solvent	Reaction steps	Yield	Ref.
1	a-MoO_3	Air	DMSO	One step	78.3%	35
2	Sulfonated MoO_3-ZrO_2	O_2	DMSO	One step	74%	36
3	MoO_x/CS-air	O_2	DMSO	One step	77.8%	37
4	f-$Ce_9Mo_1O_\delta$	O_2	DMSO	Two steps	74%	38
5	Mo-HNC	O_2	DMSO	One step	77%	39
6	β-Mo_2C@C	O_2	DMSO	Two steps	76.0%	40
7	GO	O_2	DMSO	Two steps	72.5%	49
8	Carbon nanoplatelets	O_2	DMSO	One step	70.3%	50
9	PMA-MIL-101	O_2	DMSO	One step	75.1%	51
10	MoS_2	O_2	DMSO	Two steps	81.3%	This work